Energy and Coordinates for NH_3 activation on Mo(VI)

Mo_3O_9
Energy = -879.929299 Hartree
Zero Point Energy = 19.578 kcal/mol

Coordinates:

Mo1	-2.7715344236	0.7146064886	0.9427029781
O2	-0.9923964419	0.7937090910	1.6400579775
O3	-3.4753434077	2.2639361157	0.9338472530
O4	-3.6909156518	-0.4295516919	2.1689667744
O5	-2.8125281503	0.1161653957	-0.6478620576
Mo6	-3.4532891602	-0.7350655905	4.0420428647
O7	-1.5811051949	-0.4549479899	4.3147324422
Mo8	-0.3208600847	0.6772494789	3.4271532763
O9	-4.3593847582	0.3856357133	4.9467646959
O10	-3.9442890987	-2.2951048461	4.5057236173
O11	-0.2903642210	2.2162442408	4.1525032921
O12	1.2570253261	0.0468519014	3.4801729657

NH_3

E=-56.556399 Hartree
Zero Point Energy = 21.617 kcal/mol
Coordinates:

N16	-1.4845868414	-2.7083937910	2.7915077559
H17	-1.5421853446	-1.6925042342	2.8037136183
H18	-2.1685355787	-3.0189844172	2.1050798796
H19	-1.8343429512	-3.0191376956	3.6951411765

Structure 2
Energy = -936.529582 Hartree
Zero Point Energy= 44.211 kcal/mol
Coordinates

Mo1	-2.6475097383	0.8257247646	0.8929033798
O2	-0.8959446308	1.0166910797	1.6306153503
O3	-3.4403319017	2.3334693796	0.7982289501
O4	-3.5126693232	-0.3091891494	2.1307663390
O5	-2.6161957807	0.1533595151	-0.6731000626
Mo6	-3.6039430560	-0.8112725567	3.9975866658
O7	-1.7113421977	-0.2250551068	4.2414421517

Mo8	-0.3328202979	0.7672377817	3.4436553903
O9	-4.9193487466	0.0972909152	4.6006592731
O10	-4.0483737490	-2.4603399067	3.9492995163
O11	-0.1504924860	2.2630012188	4.2489514667
O12	1.1561813940	-0.0631651588	3.5371148347
N13	-3.1233550462	-1.2198370134	6.2261709809
H14	-2.8502437116	-0.3561378261	6.6911944187
H15	-3.9306732158	-1.6112369147	6.7082683274
H16	-2.3472317799	-1.8746736015	6.3014451074

Structure TS1

Energy = -936.458499 Hartree

Zero Point Energy= 40.661 kcal/mol

Coordinates

Mo1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.9024303745
O3	1.6008709858	0.0000000000	-0.5888997426
O4	-0.8713481962	1.6364409801	-0.4648688189
O5	-0.7944151568	-1.3572743815	-0.6483985604
Mo6	-0.8593048247	3.4668753104	0.1098633225
O7	0.0449671516	2.9772641103	1.7876806651
Mo8	0.0748286460	1.5590997294	3.0266451498
O9	-0.5136896290	4.3284540526	-1.4724728464
O10	-2.4080855005	3.9420988043	0.5872833469
O11	1.4965102647	1.6105261873	3.9654257717
O12	-1.2571639924	1.6007403083	4.0891925302
N13	0.5532344312	5.1221994482	0.3808871735
H14	1.2903327141	4.8860959416	1.0438104110
H15	0.3070484400	4.9330380456	-1.0299417478
H16	0.0700041407	5.9457812292	0.7434196643

Structure 3

Energy = -936.490376 Hartree

Zero Point Energy= 42.525 kcal/mol

Coordinates

Mo1	-2.9068289827	0.9190341816	0.8981506646
O2	-1.0602501323	1.0347024067	1.4225881735
O3	-3.6399524869	2.4635422824	0.8283154463
O4	-3.6581956287	-0.0898760289	2.2759244148
O5	-3.1086311539	0.1650857805	-0.6195343159
Mo6	-3.5520809715	-0.6936759626	4.1989545358
O7	-1.6815011922	-0.1881956674	4.0640826875
Mo8	-0.3318614611	0.7830305157	3.1609417100

O9	-5.2129667549	0.2705966248	4.2718158684
O10	-3.7675493979	-2.3568399936	4.0190220997
O11	-0.0607904838	2.2765626264	3.9448842366
O12	1.1449898055	-0.0686852361	3.1177597202
N13	-3.5441417294	-0.6555089260	6.1361956144
H14	-5.4810706929	0.5863719640	3.3936393943
H15	-3.6356778621	-1.4870705537	6.7137496908
H16	-3.5271682122	0.1946068070	6.6950054708

TS2

Energy = -936.442737 Hartree

Zero Point Energy= 39.616 kcal/mol

Coordinates

Mo1	-3.0017989343	0.9726184057	1.1116924298
O2	-1.1138877539	1.0141308123	1.4508277459
O3	-3.7150454787	2.4860915616	1.4694438207
O4	-3.6375768839	-0.3064330709	2.3293453207
O5	-3.3709225870	0.5728517505	-0.5031828747
Mo6	-3.2845866290	-0.9004965603	4.1856876551
O7	-1.3954118296	-0.5789141599	3.9655733937
Mo8	-0.2426668196	0.6627163743	3.1126763782
O9	-5.1466982638	0.1615180367	4.3815351607
O10	-3.4428093318	-2.5761198303	4.2627359253
O11	-0.1460367956	2.0905332187	4.0422580983
O12	1.3340957278	0.0510014796	2.9079682213
N13	-3.5686950431	-0.2495235524	5.9183630493
H14	-5.3771233661	0.8125185881	3.7005975555
H15	-3.5275123199	-0.8548848718	6.7406624230
H16	-4.5990959587	0.3648789598	5.4499332597

Structure 4

Energy = -936.484806 Hartree

Zero Point Energy= 42.225 kcal/mol

Coordinates

Mo1	-3.0187950661	1.2572305327	1.2395316650
O2	-1.1427701634	0.9075370088	1.3707965047
O3	-3.3526536888	2.9178130180	1.4597971729
O4	-3.8121497172	0.2470712058	2.6135660191
O5	-3.6437445039	0.7964137900	-0.2815138142
Mo6	-3.3022843997	-0.6642583233	4.3280673087
O7	-1.4394486050	-0.7878597669	3.7986371667
Mo8	-0.1558493377	0.2231758736	2.8594419314
O9	-5.6407533917	-0.5209604092	4.2824731331
O10	-3.6883697420	-2.2622805298	4.7878095809

O11	0.4347857029	1.4991458844	3.8276366668
O12	1.1711734449	-0.7342884794	2.3798085164
N13	-3.2808511288	0.3836893496	5.7343162102
H14	-6.0099223149	-1.4168291578	4.2613534388
H15	-5.8237891022	-0.1074823689	3.4224664378
H16	-3.4496721592	0.2808811379	6.7365099045

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Energy = -860.038280 Hartree
Zero Point Energy: 26.172 kcal/mol
Coordinates:

Mo1	-2.8422109880	0.6708402985	0.9520967338
O2	-1.0322554050	0.7087909867	1.5730401689
O3	-3.5045761123	2.2410961270	0.9586253535
O4	-3.7359571187	-0.4376228156	2.2168110571
O5	-2.9736392953	0.0497924886	-0.6273646806
Mo6	-3.4322929483	-0.5634100064	4.1190380981
O7	-1.5077492227	-0.5385743759	4.2665046139
Mo8	-0.2665430753	0.5523789704	3.3201013156
O9	-4.1543059183	-1.9225435623	4.8375737726
O10	-0.1386370907	2.0863561916	4.0516850406
O11	1.2847635175	-0.1477344252	3.2889117075
N12	-4.0549446293	0.8938568287	4.8677771365
H13	-4.7112446783	1.1790420904	5.5959485203

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Energy = -1012.946230 hartree
Zero Point Energy (ZPE): 59.34 kcal/mol
Coordinates:

Mo1	-3.0452412081	1.2656664475	1.3714818944
O2	-1.1498917390	1.4513352035	1.5591247917
O3	-3.8523730965	2.4251924280	2.3807852903
O4	-3.4719217093	-0.4050431851	2.0224277885
O5	-3.5605894144	1.4511775522	-0.2453823908
Mo6	-3.3628558163	-1.1778050193	3.9684683117
O7	-1.8456912537	0.0971999333	4.0678446423
Mo8	-0.3425440204	0.7594893145	3.1582363097
O9	-5.1640857468	-1.6366868249	3.4613262636
O10	-2.5284704427	-2.6311254580	3.7751456025
O11	0.4422010352	1.9680564507	4.0750270442
O12	0.7913943854	-0.4599719862	2.7820486198
N13	-3.6535236684	-1.2919178043	5.8671746488
H14	-5.3085460170	-1.5726364545	2.5035163405
H15	-3.3248599625	-2.0462993716	6.4628312159
O16	-4.5747383284	0.8733434642	4.5511292634
H17	-4.0871872132	-0.5237055854	6.3726607342

H18	-5.4759121918	0.6772754367	4.2544191316
H19	-4.2793820917	1.6299482283	3.9965845835

TS3

Energy = -1012.910356 hartree

Zero Point Energy (ZPE): 55.579 kcal/mol

Coordinates:

Mo1	-2.9084264448	1.0770484726	1.1014026035
O2	-1.0377291320	1.1741201064	1.5050462469
O3	-3.6713089419	2.5911151900	1.3379006040
O4	-3.5716303243	-0.1637264128	2.3329700701
O5	-3.1963271285	0.5807459141	-0.5070954134
Mo6	-3.2723135401	-1.0621114676	4.1177816770
O7	-1.3867614873	-0.6069067650	3.8520107540
Mo8	-0.2185472106	0.6920149218	3.1629231479
O9	-5.2719929316	-0.5033356893	4.1596758748
O10	-3.2603887917	-2.7435864273	3.9968932411
O11	-0.1526441444	2.0389908011	4.2143081941
O12	1.3645688198	0.0863512789	2.9652597805
N13	-3.3738557990	-0.6566824572	5.9239464001
H14	-5.5256074218	-0.1866061484	3.2791071041
H15	-3.2152094322	-1.4238584409	6.5837442751
O16	-5.3112713216	0.8370337327	6.1479823284
H17	-4.3272198482	0.2878746124	6.2752981303
H18	-5.5109024440	0.2980124102	5.1934492880
H19	-5.9426004915	0.5690488797	6.8312163818

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Energy = -1012.927507 hartree

Zero Point Energy (ZPE): 58.27kcal/mol

Coordinates:

Mo1	-2.9974631666	1.3453509215	1.4528339755
O2	-1.0910589178	1.2879854679	1.5915112090
O3	-3.6071956221	2.8513131178	1.9844813395
O4	-3.5974431084	-0.0251718460	2.5877230910
O5	-3.5292828335	1.0947865883	-0.1506140649
Mo6	-3.0407165201	-1.1373802371	4.1597046615
O7	-1.1732590974	-0.8358032240	3.6630470289
Mo8	-0.0595669792	0.5284269902	3.0145316671
O9	-5.3042409466	-1.1215574741	4.2055241999
O10	-3.0780969616	-2.8309675911	4.2346022639
O11	0.2237004036	1.6927883466	4.2331920191

O12	1.4470480708	-0.0776369672	2.4904449152
N13	-3.1003202057	-0.4445962595	5.8038584221
H14	-5.5868420176	-0.9156188615	3.3006038630
H15	-3.0697370882	-0.9868372444	6.6727581014
O16	-5.6022769214	1.0239963008	5.6620262458
H17	-4.6724787160	1.0351122551	5.9517271346
H18	-5.5768623503	-0.3353657755	4.7692733407
H19	-6.1411513437	1.0770522026	6.4613425345

TS4

Energy = -936.404275hartree

Zero Point Energy (ZPE): 39.103 kcal/mol

Coordinates:

Mo1	-2.3624849854	0.5082737401	0.7920488987
O2	-0.8139258910	0.9863475710	1.7797386907
O3	-3.1095192372	1.8893545432	0.1312680493
O4	-3.5409496814	-0.3438690321	2.0453257785
O5	-1.9757442188	-0.5274090547	-0.5026130612
Mo6	-3.7578757233	-0.7254418812	3.9045365318
O7	-2.2986141897	0.6137364670	4.3247562242
Mo8	-0.5877345065	0.9889988276	3.6940782281
O9	-4.8929252140	0.3710744222	4.9308406274
O10	-4.4937120968	-2.3791917051	3.9467241546
O11	-0.0214616089	2.4713826176	4.3207417615
O12	0.4794243351	-0.2568139658	4.1849793307
N13	-2.5118518012	-1.8817924243	4.7592725376
H14	-1.6025841854	-1.5245807599	5.0636392943
H15	-4.5877427887	0.8716291545	5.7044598749
H16	-3.5325629242	-2.7623753715	4.4580751327

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Energy = -936.467541 hartree

Zero Point Energy (ZPE): 41.528 kcal/mol

Coordinates:

Mo1	-2.2911773204	0.4419781201	0.8907727950
O2	-0.6415893981	0.8152342269	1.7338368637
O3	-3.1287513169	1.8871241895	0.5504369828
O4	-3.3763193487	-0.7102625193	2.0173659691
O5	-2.0089466808	-0.3349917100	-0.5968643330
Mo6	-3.6728154740	-0.9287332237	3.8696511887
O7	-2.4916510350	1.0075297422	3.9165596173
Mo8	-0.7044869844	1.1653588503	3.6543360951
O9	-4.6313994629	0.2072698853	5.0271345419
O10	-4.9481531738	-2.3125741472	3.8226951743

O11	-0.1157541075	2.6937193050	4.1467374436
O12	0.0693904303	-0.1084424737	4.5431749363
N13	-2.2666500368	-1.6058598662	4.5779223754
H14	-1.2854928995	-1.5301425125	4.8952044652
H15	-4.1515729819	1.0016773526	5.3204617022
H16	-4.7526618245	-3.2084740159	4.1350088194

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Energy and Coordinates for NH3 activation on Mo(IV)

Path 1 (making H_2O)

Mo_3O_8
Energy = -804.658928 Hartree
Zero Point Energy = 16.964 kcal/mol
Coordinates:

Mo1	-2.6357114552	0.3671471486	0.8301637744
O2	-0.9301098337	0.7857648447	1.6626729115
O4	-3.7138755698	-0.4819254436	2.2066145730
O5	-3.1020271160	0.7104407725	-0.7559043126
Mo6	-3.4940102784	-0.6533005730	4.0845700837
O7	-1.6530952839	-0.2505141459	4.4206083048
Mo8	-0.3433269009	0.7699654154	3.4681903348
O9	-4.5050925123	0.4534823630	4.8965221453
O10	-3.9010328418	-2.2182757728	4.6206145932
O11	-0.2695457226	2.3615971741	4.0745706835
O12	1.2103989730	0.0864804392	3.6134212767

Structure 10
Energy = -861.273949 Hartree
Zero Point Energy = 41.972 kcal/mol
Coordinates:

Mo1	-2.8012648836	0.7396000272	1.0094101981
O2	-0.9529150256	0.7679937893	1.5265149099
O3	-3.5332386354	2.2116409537	1.5462483154
O4	-3.5561891091	-0.6058185961	2.0529903918
O5	-3.0520398150	0.5191587227	-0.6645009237
Mo6	-3.3826177292	-0.8310182461	4.0364292492
O7	-1.3880958897	-0.6573233359	4.1191405786
Mo8	-0.3491338238	0.6816709229	3.3466062240
O9	-4.1903225014	-2.0752972978	4.8531700904
O10	-0.8140544067	2.1473045065	4.1382182279

O11	1.3289027727	0.4159129581	3.5109455656
N12	-3.7274580808	1.3807236132	4.4522871178
H13	-4.0252012716	1.8617212671	3.5938063790
H14	-4.4165235038	1.5672066325	5.1798782147
H15	-2.8443023477	1.8342068925	4.7194173012

TS5

Energy = -861.244979 Hartree

Zero Point Energy = 38.074kcal/mol

Coordinates:

Mo1	-2.8097474524	0.6854133597	0.9558685664
O2	-1.0321332113	0.6731060537	1.5944275607
O3	-3.4662298382	2.2549102023	1.1870561850
O4	-3.7687862341	-0.5008986966	2.1120737798
O5	-2.9307014153	0.2583148376	-0.6918178985
Mo6	-3.3305584522	-0.8160139011	3.9698440556
O7	-1.4571554056	-0.8244598068	4.0228807818
Mo8	-0.3828471946	0.7196856717	3.4421892433
O9	-4.3190232284	-1.9157614457	4.8044445903
O10	-1.3052122215	2.0148797602	4.3291746626
O11	1.2744199722	0.4728117430	3.7411290566
N12	-3.6676266067	1.1627307862	4.5696120570
H13	-4.3142609570	1.6697884502	3.9617360946
H14	-4.0026602098	1.2586098029	5.5286947639
H15	-2.4395202271	1.7353416276	4.4742453123

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Energy = -861.250550 Hartree

Zero Point Energy = 40.099 kcal/mol

Coordinates:

Mo1	-2.8402860840	0.6908561729	0.9791995971
O2	-1.0198938691	0.7096648471	1.5714383293
O3	-3.5088836996	2.2471590317	1.2507886324
O4	-3.7044139745	-0.5411781239	2.1302093271
O5	-3.0139175745	0.2778261128	-0.6667606449
Mo6	-3.3096052136	-0.7477330605	4.0245697322
O7	-1.4164383204	-0.7149649376	4.1001495005
Mo8	-0.3029200317	0.6892469682	3.3611985617
O9	-4.2315107728	-1.9219211077	4.8363267518

O10	-0.9854760410	2.1733646112	4.3027787026
O11	1.3155864813	0.2529205830	3.6097782432
N12	-3.8131798107	1.1112837132	4.5374709241
H13	-4.4208698912	1.6353904329	3.9081441788
H14	-4.0853767190	1.2892983809	5.5022384304
H15	-1.9503041187	2.0996987037	4.4999402499

TS6

Energy =-861.232278 Hartree
Zero Point Energy = 37.589 kcal/mol
Coordinates:

Mo1	-2.7583914199	0.7585252931	1.0027549020
O2	-0.9877451086	0.4787533193	1.4973430175
O3	-3.1505794104	2.3868435207	1.4201525839
O4	-3.7729031005	-0.4193688050	2.1545638357
O5	-3.0354773818	0.4910639009	-0.6601526131
Mo6	-3.4044856004	-0.6864885761	4.0086974639
O7	-1.5782380917	-0.8833698394	4.0793709422
Mo8	-0.2796697594	0.5431302897	3.3776015768
O9	-4.3284976141	-1.9288219993	4.7086445922
O10	-1.6169020400	2.0702747122	3.9771717098
O11	1.3815951818	0.4897349485	3.6944445043
N12	-3.6611911840	0.9379631816	4.8359289176
H13	-4.3374386975	1.2065816405	5.5492301234
H14	-2.6109776078	1.6772144782	4.4672570026
H15	-1.8822777712	2.7017733758	3.2845140330

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Energy=-861.234985 Hartree
Zero Point Energy = 40.247 kcal/mol
Coordinates:

Mo1	-2.7514092292	0.7732775334	1.0164716430
O2	-0.9753622426	0.4457001409	1.4620140966
O3	-3.0561179405	2.4188903618	1.4801950651
O4	-3.7524242808	-0.3752775959	2.1709025397
O5	-3.0919321296	0.5406130885	-0.6390512944
Mo6	-3.4189500033	-0.6556853950	4.0529029068
O7	-1.5628272605	-0.8051831460	4.1548576241
Mo8	-0.2547277983	0.4887370433	3.3395100042
O9	-4.3074311602	-1.9471407679	4.7118363621
O10	-1.6010718147	2.1694399681	3.8480353244
O11	1.4055354948	0.3505333547	3.6209171438
N12	-3.7948709055	0.8997014206	4.8836029416

H13	-4.5026663954	1.1091823439	5.5892385733
H14	-2.3971255962	1.8902749584	4.3978446226
H15	-1.9964652653	2.6230237911	3.0679769503

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Energy =-784.765378 Hartree
Zero Point Energy = 23.546 kcal/mol
Coordinates:

Mo1	-2.7815895220	0.9010434805	1.0305925252
O2	-0.9632657409	0.6759885143	1.5328202629
O3	-3.2234768597	2.5443967133	1.1756914536
O4	-3.7689921173	-0.1664144364	2.2615010826
O5	-3.0636795414	0.4156132784	-0.5800127983
Mo6	-3.4610271156	-0.5234025466	4.1335772172
O7	-1.5556395042	-0.6309090144	4.2954038668
Mo8	-0.1473031880	0.1351120865	3.2138231017
O9	-4.2605174395	-1.9263589633	4.6692080088
O11	1.4815528603	0.3006238146	3.6396856704
N12	-4.0220060894	0.8561235572	5.0675930281
H13	-4.7016106277	1.0420161225	5.8060800194

<u>Path 2 (making 2OH on different Mo sites)</u>

TS7

Energy = -861.2202136 Hartree
Zero Point Energy = 35.951 kcal/mol
Coordinates:

Mo1	-2.8585794121	0.7197502098	1.0063130592
O2	-1.0759215325	0.9014781694	1.7316369558
O3	-3.9559799566	1.9142239328	1.8356373203
O4	-3.3519760286	-0.8536982870	2.0780926480
O5	-2.9295214853	0.4586755509	-0.6771363476
Mo6	-3.4249441298	-0.6693865678	3.9330471261
O7	-1.6293666388	-0.2708167253	4.3589883931
Mo8	-0.2082676859	0.6650726040	3.4157725776
O9	-4.0605662892	-1.9750349152	4.8169285361
O10	0.0665988358	2.3653972627	4.2260870554
O11	1.1330528114	-0.3635875717	3.3099797344
N12	-4.4098728060	0.8945636388	4.0684513992
H13	-4.2256325674	1.5940969460	2.9546062890
H14	-5.2351821198	1.0450054180	4.6493543209
H15	-0.6519720421	2.9713095194	4.4622769027

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Energy = -861.230218 Hartree
Zero Point Energy = 38.463 kcal/mol
Coordinates:

Mo1	-2.8731576287	0.7081690977	0.8634402169
O2	-1.1845277284	0.9905195719	1.7509099002
O3	-3.7896272970	2.3638836477	0.7038058310
O4	-3.7169101104	-0.3861970642	2.1955506212
O5	-2.6030071655	-0.1910543377	-0.5461441826
Mo6	-3.3325224449	-0.6743827714	4.0499360174
O7	-1.4387998918	-0.7919267009	4.0393129741
Mo8	-0.3337238634	0.6696130487	3.4340645212
O9	-4.1395748132	-2.0152142445	4.7213699502
O10	-0.8176950147	2.0323428194	4.6601254641
O11	1.2779211616	0.1453141785	3.3782788654
N12	-3.7065671568	0.8543182332	4.9097220192
H13	-4.3348638959	1.0021525327	5.7027090700
H14	-1.7446656970	1.9911738796	4.9741136798
H15	-3.9768613028	2.9493101217	1.4537494963

Path 3 (making 2OH on same Mo)

TS2 (H from OH to oxo) E=-861.154432
Zero Point Energy = 38.074kcal/mol
Coordinates:

H_2O assisted TS2

19
Energy =-937.693406 Hartree
Zero Point Energy = 54.595kcal/mol
Coordinates:

Mo1	-2.6001942891	0.7731996306	0.9364595176
O2	-0.8882768645	0.5510358620	1.7144765706
O3	-3.1285196014	2.3938763012	1.1589602565
O4	-3.6515112325	-0.3739280656	2.0164793522
O5	-2.6339041054	0.3477539449	-0.7214721461
Mo6	-3.7645456364	-0.5664983969	3.9329818933
O7	-1.9294229347	-0.1691573844	4.3634783231
Mo8	-0.2725779544	0.3528839710	3.5329476731

O9	-4.1481926136	-2.1669684229	4.3477862103
O10	0.2305242532	2.0361576780	4.1973140620
O11	0.8448194472	-0.9308874259	3.5512614426
N12	-4.9186866766	0.8291788153	4.6292564699
H13	-4.8598867874	1.8119853670	4.3713542240
H14	-5.7190239809	0.6521555273	5.2295680341
H15	1.1790710030	2.1484070339	4.4744317423
O16	2.8721420130	2.0306632826	4.7126344810
H17	3.3711112589	2.3125742048	3.9346232148
H18	3.1616900488	1.1257296948	4.8902870729

TS8b

Energy =-937.667527 Hartree
Zero Point Energy = 53.501 kcal/mol
Coordinates:

Mo1	-2.7063537997	0.6778846026	0.8814235330
O2	-0.9772643124	0.6123642439	1.6607704872
O3	-3.2974793282	2.2914561251	0.8903425520
O4	-3.6875813168	-0.3636222908	2.1209004375
O5	-2.7451223702	0.0258519287	-0.7019709853
Mo6	-3.6326724627	-0.6187488240	4.0336227575
O7	-1.8132966375	-0.0466612446	4.3692525317
Mo8	-0.2734707168	0.6349248053	3.4495156722
O9	-3.8224061549	-2.2657002401	4.4021053615
O10	0.1513155312	2.2583365786	4.0371614159
O11	1.1830520753	-0.3591234330	3.6491147886
N12	-4.8773311080	0.6287065054	4.8561895134
H13	-4.9836299312	1.6059755411	4.5942202547
H14	-5.5955475891	0.3462474785	5.5167899185
H15	1.5607172489	2.0865573049	4.3903196728
O16	2.4984522353	1.5675722746	4.5205459966
H17	2.1413422212	0.6102264300	4.1692879355
H18	2.7148026449	1.5109955123	5.4638833368

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Energy =-937.693001 Hartree
Zero Point Energy = 54.429 kcal/mol
Coordinates:

Mo1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.8940059000
O3	1.6505800200	0.0000000000	-0.6671920231
O4	-0.8989690909	1.7205281153	-0.3583647686
O5	-0.9057825036	-1.3988363885	-0.5907519171
Mo6	-2.1918052888	2.7780750893	0.7554415376

O7	-1.4755794204	2.4088999219	2.5118061017
Mo8	-0.2121833815	1.2301877425	3.3592800987
O9	-3.8150682125	2.1594262694	0.6341378776
O10	1.2478514321	2.0820664711	3.5547206809
O11	-1.0413342543	0.3617206946	4.8026768632
N12	-1.8907547686	4.7031123227	0.3763749918
H13	-0.9509010953	5.1873511862	0.3512953820
H14	-2.6402040096	5.3631728796	0.1478613484
H15	-0.9819615585	0.4791850725	7.9419980391
O16	-0.2050568933	0.4398126980	7.3450765248
H17	-0.7101954671	0.3885733666	5.7414797331
H18	0.3016436497	-0.3625025270	7.6091104097

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Energy =-861.255036 Hartree
Zero Point Energy = 39.302kcal/mol
Coordinates:

Mo1	-2.6746601429	0.5107320788	0.8142131601
O2	-0.9681506758	0.5886883478	1.6442384302
O3	-3.1198544125	2.0101708717	0.1195110342
O4	-3.7933366849	0.0933029978	2.2839218197
O5	-2.7125808356	-0.7092127347	-0.3859047566
Mo6	-3.6080759485	-0.4339662125	4.1311546621
O7	-1.7932719972	0.1646240334	4.4109018791
Mo8	-0.2593718861	0.7584493772	3.4253543895
O9	-3.6671647026	-2.1257891729	4.2625461387
O10	0.0067467194	2.4062545114	3.7287765414
O11	1.1917370226	-0.4422488018	3.6650276260
N12	-4.8142996187	0.5930629206	5.2501063675
H13	-4.9297297410	1.6031248050	5.2069250187
H14	-5.4521802696	0.1783239385	5.9235765194
H15	1.1746414671	-1.3629623668	3.3602917004

TS9

Energy = -861.218142 Hartree
Zero Point Energy = 36.93kcal/mol
Coordinates:

Mo1	-2.7959483285	0.6309438709	0.8813618338
O2	-1.1414906503	1.1700839803	1.6032521467
O3	-3.5048519001	1.8918882839	-0.0243214330
O4	-3.9181315327	0.1234968051	2.3735648687
O5	-2.5744308130	-0.7029726028	-0.1613413538
Mo6	-3.2936840439	-0.6001165862	4.0207863517
O7	-1.5041031033	-0.8510817796	3.6826030000

Mo8	-0.3989281513	0.8275149493	3.3936227784
O9	-4.1415562336	-1.9829892343	4.5246808048
O10	-1.2020626782	1.8601253683	4.6490584111
O11	1.2580899719	0.0164075435	3.8796743390
N12	-3.3099399782	0.7268366859	5.3064376082
H13	-3.8271973402	0.7688937082	6.1834181028
H14	-2.2829080023	1.4287009536	5.1093114074
H15	1.2802307043	-0.8933128675	4.2152002878

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Energy = -861.229559 Hartree
Zero Point Energy = 39.302 kcal/mol
Coordinates:

Mo1	-2.7772269859	0.5765297829	0.8997964922
O2	-1.1343249828	1.2188316688	1.6402834957
O3	-3.4782859541	1.7493998507	-0.1214467218
O4	-3.9308607861	0.1620597021	2.3546119138
O5	-2.4779274557	-0.8189870291	-0.0380759631
Mo6	-3.3616190458	-0.5555464901	4.0626883046
O7	-1.5088758810	-0.6940117651	3.7898190165
Mo8	-0.3512200799	0.8477266829	3.3637026897
O9	-4.1105381984	-2.0169725348	4.5093232339
O10	-0.9309661454	1.9968084905	4.7388638846
O11	1.2773503364	-0.1013839409	3.5831821653
N12	-3.6137916566	0.6953586550	5.3109348178
H13	-4.1673348188	0.6680514295	6.1697906819
H14	-1.7560348203	1.7480114375	5.2118948583
H15	1.2387720640	-1.0381874501	3.8370783693